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Orthogonal localized wave functions of an electron in a magnetic field

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Abstract

We prove the existence of a set of two-scale magnetic Wannier orbitals, $w_{mn}(\mathbf{r})$, in the infinite plane. The quantum numbers of these states are the positions (m, n) of their centers which form a von Neumann lattice. Function $w_{00}(\mathbf{r})$ localized at the origin has a nearly Gaussian shape of $\exp(-r^2/4l^2)/\sqrt{2\pi}$ for $r \lesssim \sqrt{2\pi}l$, where l is the magnetic length. This region makes a dominating contribution to the normalization integral. Outside this region function, $w_{00}(\mathbf{r})$ is small, oscillates, and falls off with the Thouless critical exponent for magnetic orbitals, r^{-2} . These functions form a convenient basis for many electron problems.

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I. INTRODUCTION

Computational methods for interacting electrons in a strong magnetic field have been developing rapidly in the last decade.¹ They employ different geometries which suggest different sets of single-electron wave functions and quantum numbers of many-electron states. The toroidal geometry was advanced by Yoshioka, Halperin, and Lee.² The symmetry classification of the many-electron functions in this geometry was proposed by Haldane.³ Afterwards most of the finite-size computations were performed in the framework of the spherical geometry proposed and developed by Haldane and Rezayi.⁴

Landau functions, eigenfunctions of angular momentum, and localized functions called coherent states⁵⁻⁷ are usually used in the plane geometry. Localized functions have obvious advantages as applied to the Wigner crystal theory and also to some systems with strongly inhomogeneous potential distribution. We expect that these functions may also be effective as the basis functions for numerical diagonalization. Since the matrix size increases exponentially with the number of particles, N , this number is strongly restricted by computational facilities, e.g., by $N \leq 10$ for the filling factor $\nu = 1/3$. Therefore, it seems tempting to develop some procedure for a strong reduction of the dimension of the Hilbert space by eliminating functions which make only a small contribution to the low-energy states. We believe that the prospects for such an approach are promising since the correlation energy, $\varepsilon_{\text{corr}}$, which can be evaluated by the magnitude of the Laughlin gap or by the energy difference between the liquid and solid phases, is small compared with the characteristic Coulomb energy, $\varepsilon_C = e^2/\epsilon l$, where $l = (c\hbar/eB)^{1/2}$ is the magnetic length. The inequality $\varepsilon_{\text{corr}} \ll \varepsilon_C$ implies that the subspace chosen for diagonalization can be restricted by the electron configurations with low Hartree-Fock energies. Such an approach has been recently developed and successfully applied to electrons on a lattice.⁸

As a first step in developing a low-energy states selecting procedure, one should construct a basis of localized, particle-like functions with a characteristic size about l . However, some general requirements exclude the existence of a complete system of single-electron states

which are both exponentially localized and linearly independent. This point should be explained in more detail.

The coherent states⁹ on a von Neumann lattice are the most localized eigenfunctions for an electron in a magnetic field. For such a lattice, with a single flux quantum per a unit cell, the area of a unit cell equals $2\pi l^2$. The set of coherent states, $c_{mn}(\mathbf{r})$, of the lowest Landau level (LLL) can be obtained by the magnetic translations of the function $c_{00}(r) = \exp(-r^2/4l^2)/\sqrt{2\pi}$ from the origin to all lattice sites, (m, n) . The set $c_{mn}(\mathbf{r})$ is complete, i.e., an arbitrary function belonging to the LLL can be expanded in functions $c_{mn}(\mathbf{r})$. This statement is physically appealing and is supported by a rigorous mathematical proof.^{10,11} The functions $c_{mn}(\mathbf{r})$ are obviously non-orthogonal. A straightforward way to orthogonalize such a set is to transform it into the Bloch representation, and then go back to the site representation. Wannier applied this procedure to a one-dimensional chain of Gaussians.¹² If the functions $c_{mn}(\mathbf{r})$ were linearly independent, this orthogonalization procedure would result in a set of exponentially localized functions. However, Perelomov¹⁰ has established a non-trivial fact that the set $c_{mn}(\mathbf{r})$ is actually overcomplete by exactly one function and presented the explicit form of the linear equation relating these functions; see Eq. (4) below. The overcompleteness of the set $c_{mn}(\mathbf{r})$ imposes hard restrictions on the localization of Wannier functions. Zak and collaborators^{13,14} have shown that the exponential localization and the orthogonality of magnetic orbitals are incompatible. Thouless¹⁵ proved even a stronger result by relating the localization of magnetic orbitals to the existence of the Hall current. He showed that in systems supporting a Hall current the orbitals should fall off with distance no faster than by the inverse-square law, hence, r^{-2} is a critical exponent.

Having in mind these restrictions on the falloff of magnetic orbitals, one can question whether particle-like orbitals suitable for restricted-basis finite-size calculations do exist. It is the main result of this paper that a set of two-scale orbitals $w_{mn}(\mathbf{r})$, which satisfy the above requirements exists.¹⁶ In the small \mathbf{r} region, $r \lesssim \sqrt{2\pi}l$, the orbital $w_{00}(\mathbf{r})$ is very close to the Gaussian $c_{00}(r)$, and this region contributes about 95% to the normalization integral. For $r \gtrsim \sqrt{2\pi}l$, the function $w_{00}(\mathbf{r})$ falls off as r^{-2} in exact correspondence with

the Thouless criterion and shows an oscillatory behavior which ensures orthogonality to the different orbitals $w_{mn}(\mathbf{r})$.

The term Wannier functions is usually applied only to the orbitals which fall off exponentially. Since the functions $w_{mn}(\mathbf{r})$ are normalizable and have a well localized Gaussian core, we shall term them as Wannier functions in what follows.

The paper is organized as follows. In Sec. II general equations are presented and the behavior of magnetic Bloch functions near the singular point in the momentum plane is studied. It is of importance for establishing the completeness of the sets of Bloch and Wannier functions. The basic results are discussed in Sec. III where two-scale Wannier functions $w_{mn}(\mathbf{r})$ of the infinite plane are derived and studied analytically and numerically. In Sec. IV some results for Wannier functions on the finite plaquettes are presented. The results are summarized in Conclusion.

II. GENERAL EQUATIONS

Let us choose a rectangular unit cell with sides \mathbf{a} and \mathbf{b} such that $ab = 2\pi$ and a normalization plaquette with sides $L_x = \alpha a$ and $L_y = \beta b$, where α and β are integers. Here and below $l = 1$. It is convenient to define the function $c_{mn}(\mathbf{r})$ centered at a site (m, n) as

$$c_{mn}(\mathbf{r}) = T_{m\mathbf{a}}T_{n\mathbf{b}} c_{00}(r) , \quad c_{00}(r) = \exp(-r^2/4)/\sqrt{2\pi} , \quad (1)$$

where $T_{m\mathbf{a}}$ and $T_{n\mathbf{b}}$ are operators of magnetic translations¹⁷ along \mathbf{a} and \mathbf{b} axes, and $c_{mn}(\mathbf{r})$ are the eigenfunctions of the Schroedinger equation of an electron in a magnetic field. The axial gauge $\mathbf{A}(\mathbf{r}) = \frac{1}{2} \hat{\mathbf{z}} \times \mathbf{r}$ is used. The general definition of the operator $T_{\mathbf{R}}$ for a particle with a charge $e > 0$ is:

$$T_{\mathbf{R}}\psi(\mathbf{r}) = \exp\left\{-\frac{i}{2} \mathbf{R} \cdot \mathbf{A}(\mathbf{R})\right\} \exp\{i\mathbf{r} \cdot \mathbf{A}(\mathbf{R})\} \psi(\mathbf{r} - \mathbf{R}) . \quad (2)$$

Therefore, the explicit form of the function $c_{mn}(\mathbf{r})$ is:

$$c_{mn}(\mathbf{r}) = (-)^{mn} \exp\left\{-\frac{1}{4}(\mathbf{r} - \mathbf{R}_{mn})^2 + \frac{i}{2} \hat{\mathbf{z}} \cdot (\mathbf{R}_{mn} \times \mathbf{r})\right\}/\sqrt{2\pi} , \quad (3)$$

where $\mathbf{R}_{mn} = m\mathbf{a} + n\mathbf{b}$.

The set of functions $c_{mn}(\mathbf{r})$ obeys the Perelomov overcompleteness equation¹⁰

$$\sum_{mn=-\infty}^{\infty} (-)^{m+n} c_{mn}(\mathbf{r}) = 0 \quad (4)$$

Therefore functions $c_{mn}(\mathbf{r})$ are linearly dependent.

The operators $T_{m\mathbf{a}}T_{n\mathbf{b}}$ in Eq. (1) are considered as elements of the outer Kronecker product $G_{\mathbf{a}} \otimes G_{\mathbf{b}}$ of the groups $G_{\mathbf{a}}$ and $G_{\mathbf{b}}$ of the magnetic translations along \mathbf{a} and \mathbf{b} . It follows from Eq. (2) that $T_{\mathbf{a}}T_{\mathbf{b}} = T_{\mathbf{b}}T_{\mathbf{a}}e^{iab} = T_{\mathbf{b}}T_{\mathbf{a}}$. Therefore, $T_{m\mathbf{a}}$ and $T_{n\mathbf{b}}$ commute for arbitrary values of m and n . By definition,¹⁸ the outer product consists of operators $T_{m\mathbf{a}}T_{n\mathbf{b}}$ and does not include operators $T_{m\mathbf{a}+n\mathbf{b}}$ with $mn \neq 0$ which do not commute with the operators of the $T_{m\mathbf{a}}$ and $T_{n\mathbf{b}}$ types. Therefore, the Kronecker product $G_{\mathbf{a}} \otimes G_{\mathbf{b}}$ forms an Abelian group of translations, and one can introduce a two-dimensional momentum \mathbf{k} and follow the Wannier procedure.¹²

Transformation of the set $c_{mn}(\mathbf{r})$ to the momentum representation results in Bloch functions:

$$\Psi_{\mathbf{k}}(\mathbf{r}) = \sum_{mn=-\infty}^{\infty} c_{mn}(\mathbf{r}) \exp(i\mathbf{k}\mathbf{R}_{mn}) / \sqrt{\alpha\beta \nu(\mathbf{k})} . \quad (5)$$

Functions $\Psi_{\mathbf{k}}(\mathbf{r})$ with different values of \mathbf{k} are orthogonal since they belong to different irreducible representations of the group $G_{\mathbf{a}} \otimes G_{\mathbf{b}}$. Values of \mathbf{k} can be found from the boundary conditions for $\Psi_{\mathbf{k}}(\mathbf{r})$. The latter can be chosen either as regular periodic boundary conditions with respect to the magnetic translations with periods L_x and L_y , or from ϕ -periodic conditions when some twist $\phi = (\phi_x, \phi_y)$ is added.¹⁹ Therefore, the components of \mathbf{k} can take values

$$k_x = (2\pi s_x + \phi_x)/L_x, \quad k_y = (2\pi s_y + \phi_y)/L_y \quad (6)$$

inside the Brillouin zone. Here components s_x and s_y of the vector $\mathbf{s} = (s_x, s_y)$ are integers, $s_x, s_y = 0, \pm 1, \dots$, taking α and β values, respectively. Normalization coefficient $\nu(\mathbf{k})$ is determined by the equation

$$\nu(\mathbf{k}) = \sqrt{2\pi} \sum_{mn=-\infty}^{\infty} c_{mn}(0,0) \cos(\mathbf{k}\mathbf{R}_{mn}) . \quad (7)$$

The inverse Fourier transformation

$$W_{mn}(\mathbf{r}) = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}(\mathbf{r}) \exp(-i\mathbf{k}\mathbf{R}_{mn}) / \sqrt{\alpha\beta} \quad (8)$$

results in a set of orthonormal Wannier-type functions:

$$W_{mn}(\mathbf{r}) = \sum_{m'n'=-\infty}^{\infty} K_{\phi}(m' - m, n' - n) c_{m'n'}(\mathbf{r}) , \quad (9)$$

where

$$K_{\phi}(m, n) = \frac{1}{\alpha\beta} \sum_{\mathbf{k}} \exp(i\mathbf{k}\mathbf{R}_{mn}) / \sqrt{\nu(\mathbf{k})} . \quad (10)$$

The functions $K_{\phi}(m, n)$ and $W_{mn}(\mathbf{r})$ obey the equations $K_{\phi}(m + M\alpha, n + N\beta) = K_{\phi}(m, n) \exp\{i\phi(M, N)\}$, and

$$W_{m+M\alpha, n+N\beta}(\mathbf{r}) = W_{mn}(\mathbf{r}) \exp\{-i\phi(M, N)\} , \quad (11)$$

where $\phi(M, N) = M\phi_x + N\phi_y$, and M and N are integers. Therefore, $|W_{mn}(\mathbf{r})|$ is periodic with periods L_x and L_y for any value of the flux ϕ .

The above equation for the Bloch functions $\Psi_{\mathbf{k}}(\mathbf{r})$ is known both in Landau²⁰⁻²² and coherent function²³ bases, and the equation for $W_{mn}(\mathbf{r})$ was discussed more recently as applied to finite plaquettes.⁶ These equations have their analogs in the mixed kq representation.¹⁴

Functions $\Psi_{\mathbf{k}}(\mathbf{r})$ are orthogonal and, therefore, linearly independent. If they exist for any momenta $\mathbf{k} = (k_x, k_y)$, defined by Eq. (6), then the set $\Psi_{\mathbf{k}}(\mathbf{r})$ is complete. Hence, the set $W_{mn}(\mathbf{r})$ is complete, too. However, the properties of one of the functions $\Psi_{\mathbf{k}}(\mathbf{r})$, namely the function $\Psi_{\mathbf{k}_0}(\mathbf{r})$, where \mathbf{k}_0 is the corner of the Brillouin zone, need a special deliberation. At this point $k_x a = \pm k_y b = \pm \pi$, and the exponent in Eq. (5) equals $(-)^{m+n}$. Therefore, the numerator of $\Psi_{\mathbf{k}_0}(\mathbf{r})$ turns into zero because of Eq. (4). If one puts $\Psi_{\mathbf{k}_0}(\mathbf{r}) = 0$ and excludes this function from the set $\Psi_{\mathbf{k}}(\mathbf{r})$, the set becomes incomplete since it lacks a function of the translation symmetry of \mathbf{k}_0 . This problem was emphasized by Thouless.¹⁵

Since functions $\Psi_{\mathbf{k}}(\mathbf{r})$ are normalized, the denominator of $\Psi_{\mathbf{k}_0}(\mathbf{r})$ also turns into zero, $\nu(\mathbf{k}_0) = 0$. Indeed, for $\mathbf{k} = \mathbf{k}_0$ the cosine in Eq. (7) equals $\cos(\mathbf{k}_0 \mathbf{R}_{mn}) = (-)^{m+n}$, and therefore $\nu(\mathbf{k}_0) = 0$ due to Eq. (4). Function $\nu(\mathbf{k})$ is shown in Fig. 1 for a square lattice, $a = b = \sqrt{2\pi}$. One can see that $\nu(\mathbf{k})$ is positive, $\nu(\mathbf{k}) > 0$, inside the Brillouin zone and reaches its minima, $\nu(\mathbf{k}_0) = 0$, in the corners of it. Both the numerator and denominator of $\Psi_{\mathbf{k}}(\mathbf{r})$ have the order of magnitude of $|\zeta|$ when $\zeta \equiv \mathbf{k} - \mathbf{k}_0 \rightarrow 0$. The leading term in the numerator of $\Psi_{\mathbf{k}}(\mathbf{r})$ depends on φ_{ζ} , the azimuth of ζ , as it is shown below; cf. Eq. (16). On the contrary, the function $\sqrt{\nu(\mathbf{k})}$, which is the denominator of $\Psi_{\mathbf{k}}(\mathbf{r})$, is isotropic near \mathbf{k}_0 for a square lattice. Therefore, the function $\Psi_{\mathbf{k}}(\mathbf{r})$ retains the dependence on φ_{ζ} even in the limit $\zeta \rightarrow 0$. Hence, it is singular at the point $\mathbf{k} = \mathbf{k}_0$, and the limit $\Psi_{\mathbf{k} \rightarrow \mathbf{k}_0}$ does not exist.

To find the form of $\Psi_{\mathbf{k}}(\mathbf{r})$ in the limit $\mathbf{k} \rightarrow \mathbf{k}_0$, one can expand the numerator of $\Psi_{\mathbf{k}_0+\zeta}(\mathbf{r})$ in ζ and take into account Eq. (4). Then

$$\Psi_{\mathbf{k}_0+\zeta}(\mathbf{r}) = \frac{i}{[\alpha\beta\nu(\mathbf{k})]^{1/2}} \sum_{mn=-\infty}^{\infty} (-)^{m+n} \zeta \cdot \mathbf{R}_{mn} c_{mn}(\mathbf{r}) . \quad (12)$$

If one introduces complex variables $z = x + iy$ and $Z_{mn} = X_m + iY_n$, the condition (4) takes the form:

$$\sum_{mn=-\infty}^{\infty} (-)^{mn+m+n} \exp\left\{-\frac{1}{4}\mathbf{R}_{mn}^2 + \frac{1}{2}z\bar{Z}_{mn}\right\} = 0 . \quad (13)$$

Here and below complex conjugate variables are designated by bars. Since this equation is valid for arbitrary values of z and the sum converges exponentially, one can take the derivative over z :

$$\sum_{mn=-\infty}^{\infty} (-)^{m+n} \bar{Z}_{mn} c_{mn}(\mathbf{r}) = 0 . \quad (14)$$

If one takes advantage of the relation $\zeta \cdot \mathbf{R}_{mn} = (Z_{mn}\bar{\zeta} + \bar{Z}_{mn}\zeta)/2$, where $\zeta = \zeta_x + i\zeta_y$, and plugs Eq. (14) into Eq. (12), the latter takes the form:

$$\Psi_{\mathbf{k}_0+\zeta}(\mathbf{r}) \approx \frac{i/2}{[\alpha\beta\nu(\mathbf{k})]^{1/2}} \bar{\zeta} \sum_{mn=-\infty}^{\infty} (-)^{m+n} Z_{mn} c_{mn}(\mathbf{r}) . \quad (15)$$

Since $\nu(\mathbf{k})^{1/2} \propto |\zeta|$ for $|\zeta| \rightarrow 0$, Eq. (15) can be rewritten as

$$\Psi_{\mathbf{k}_0+\boldsymbol{\zeta}}(\mathbf{r}) \approx e^{-i\varphi\zeta} \Phi_{\mathbf{k}_0}(\mathbf{r}) , \quad (16)$$

where $\Phi_{\mathbf{k}_0}(\mathbf{r})$ is a regular function of \mathbf{r} possessing the symmetry of the point \mathbf{k}_0 .

Therefore, nonanalytic function $\Psi_{\mathbf{k}_0+\boldsymbol{\zeta}}(\mathbf{r})$ factors near the singular point into the product of two functions, $e^{-i\varphi\zeta}$ and $\Phi_{\mathbf{k}_0}(\mathbf{r})$. The first factor absorbs the nonanalytic dependence of $\Psi_{\mathbf{k}_0+\boldsymbol{\zeta}}(\mathbf{r})$ on $\boldsymbol{\zeta}$, whereas the second factor does not depend on $\boldsymbol{\zeta}$ and possesses the translational symmetry of the point \mathbf{k}_0 . Function $\Phi_{\mathbf{k}_0}(\mathbf{r})$, taken with an arbitrary phase factor, can be used as a Bloch function with the \mathbf{k}_0 symmetry. Therefore, Bloch functions are defined for all \mathbf{k} values. This statement concludes the proof of the completeness of the set $\Psi_{\mathbf{k}}(\mathbf{r})$. The set $W_{mn}(\mathbf{r})$ obtained from it by the orthogonal transformation of Eq. (8) is also complete.

There exists another way to construct the function $\Phi_{\mathbf{k}_0}(\mathbf{r})$. It is based on the properties of Bloch functions constructed from different sets of localized orbitals. Instead of $c_{00}(r)$, one can use the function $c_{00}^{(1)}(\mathbf{r}) = z c_{00}(r)/\sqrt{2}$ to generate the sets of orbitals $c_{mn}^{(1)}(\mathbf{r})$ and Bloch functions $\Psi_{\mathbf{k}}^{(1)}(\mathbf{r})$. The sets $c_{mn}(\mathbf{r})$ and $c_{mn}^{(1)}(\mathbf{r})$ belong to the LLL. Both sets are overcomplete and can be expanded one in another. Consequently, functions $\Psi_{\mathbf{k}}(\mathbf{r})$ and $\Psi_{\mathbf{k}}^{(1)}(\mathbf{r})$ can differ only in \mathbf{r} independent phase factors for arbitrary value of \mathbf{k} . Boon *et al.* have shown²⁴ that \mathbf{k}_0 is a regular point for the set $\Psi_{\mathbf{k}}^{(1)}(\mathbf{r})$. Therefore, one can use $\Psi_{\mathbf{k}_0}^{(1)}(\mathbf{r})$ as a function $\Phi_{\mathbf{k}_0}(\mathbf{r})$. The shape of the function $W_{mn}(\mathbf{r})$ depends on the choice of the phase of $\Phi_{\mathbf{k}_0}(\mathbf{r})$.

The properties of Bloch functions discussed in the previous paragraph can be also understood from a more general point of view. It follows from Eqs. (3) and (13) that functions $c_{mn}^{(1)}(\mathbf{r})$ can be obtained as

$$c_{mn}^{(1)}(\mathbf{r}) = \sqrt{2} \left(\partial/\partial \bar{Z}_{mn} - \frac{1}{4} Z_{mn} \right) c_{mn}(\mathbf{r}) .$$

Therefore, functions $c_{mn}^{(1)}(\mathbf{r})$ and $c_{mn}(\mathbf{r})$ belong to the same Landau level because of the existence of continuous group of magnetic translations. The same is true for the functions $c_{mn}^{(q)}(\mathbf{r})$ originating from the function $c_{00}^{(q)}(\mathbf{r}) \propto z^q c_{00}(\mathbf{r})$, where q is an arbitrary integer. Bloch

functions $\Psi_{\mathbf{k}}^{(q)}(\mathbf{r})$, constructed from them, are completely determined by the translational symmetry up to the phase factors depending only on q and \mathbf{k} . Therefore, all functions $\Psi_{\mathbf{k}}^{(q)}(\mathbf{r})$ with the same value of the momentum \mathbf{k} and different values of q coincide up to these phase factors. Singularities of functions $\Psi_{\mathbf{k}}^{(q)}(\mathbf{r})$ ensure the existence of the Hall current,¹⁵ hence, they are present for each set of functions $\Psi_{\mathbf{k}}^{(q)}(\mathbf{r})$ and can not be eliminated. However, the number of singular points and their positions in the Brillouin zone change depending on q .²⁴

It is known that the overcompleteness equation (4) is related to the properties of Jacobi $\vartheta(u|\tau)$ functions.^{10,15} Eq. (7) for $\nu(\mathbf{k})$ takes a simple form when rewritten in terms of these functions. If one performs the summation over n in Eq. (7) using the Jacobi imaginary transformation of theta functions,²⁵ $\nu(\mathbf{k})$ acquires the form:

$$\nu(\mathbf{k}) = \frac{a}{\sqrt{\pi}} e^{-k_y^2} \vartheta_3\left(\frac{a}{2\pi}k_+ \mid i\frac{a}{b}\right) \vartheta_3\left(\frac{a}{2\pi}k_- \mid i\frac{a}{b}\right), \quad (17)$$

where $k_{\pm} = k_x \pm ik_y$. The zeros of $\vartheta_3(u|\tau)$ can be found from the condition $u = (M + \frac{1}{2}) + (N + \frac{1}{2})\tau$, where M and N are integers, and one immediately recovers that the corner of the Brillouin zone, $\mathbf{k}_0 = (\pm\pi/a, \pm\pi/b)$, is a zero of $\nu(\mathbf{k})$.

III. WANNIER FUNCTIONS IN THE INFINITE PLANE

Equations (9) and (10) can be used to find Wannier functions $w_{mn}(\mathbf{r})$ localized in the infinite \mathbf{r} plane. In the limit $\alpha, \beta \rightarrow \infty$, the sum in Eq. (10) transforms into the integral over the Brillouin zone:

$$K_{\infty}(m, n) = ab \int_{(B.Z.)} \frac{d\mathbf{k}}{(2\pi)^2} \frac{\exp(i\mathbf{k}\mathbf{R}_{mn})}{\sqrt{\nu(\mathbf{k})}}. \quad (18)$$

The kernel $K_{\infty}(m, n)$ is obviously independent of ϕ .

The asymptotic behavior of $K_{\infty}(m, n)$ for $|m|, |n| \gg 1$ can be found analytically. It is determined by the behavior of the integrand near its pole, i.e., by the expansion of $\nu(\mathbf{k})$ near \mathbf{k}_0 . For a square lattice, $a = b = \sqrt{2\pi}$, this expansion has the form

$$\nu(\mathbf{k}_0 + \boldsymbol{\zeta}) \approx \gamma a^2 \boldsymbol{\zeta}^2 / 2, \quad (19)$$

where $\gamma \approx 0.5814$ is given by the series:

$$\gamma = - \sum_{mn=-\infty}^{\infty} (-)^{mn+m+n} m^2 \exp[-\frac{\pi}{2}(m^2 + n^2)]. \quad (20)$$

Substituting (19) into (18) results in the leading term of the expansion of $K_{\infty}(m, n)$ in R_{mn}^{-1} :

$$K_{\infty}(m, n) \approx (-)^{m+n} 2 \sqrt{\frac{\pi}{\gamma}} \int_{-\infty}^{\infty} \frac{d\zeta}{(2\pi)^2} \frac{\exp(i\zeta \mathbf{R}_{mn})}{\zeta} = \frac{(-)^{m+n}}{\sqrt{\pi\gamma} R_{mn}}. \quad (21)$$

The next term of this expansion falls off as R_{mn}^{-3} . An equation equivalent to $K_{\infty}(m, n) \propto (-)^{m+n}/R_{mn}$ was derived by Sen and Chitra²⁶ using a different procedure.

The asymptotic behavior of $w_{mn}(\mathbf{r})$ for large $|\mathbf{r} - \mathbf{R}_{mn}|$ values follows from Eqs. (9) and (21). The right hand side of the equation

$$w_{00}(\mathbf{r}) = \sum_{mn=-\infty}^{\infty} K_{\infty}(m, n) c_{mn}(\mathbf{r}) \quad (22)$$

for the function $w_{00}(\mathbf{r})$ includes the product of the kernel $K_{\infty}(m, n)$, whose denominator depends on m and n slowly, and the factor $c_{mn}(\mathbf{r})$, which depends on m and n exponentially for a fixed value of \mathbf{r} . One can use the asymptotic form of the kernel $K_{\infty}(m, n)$, Eq. (21), and neglect the higher order corrections to it. If one substitutes the expansion

$$R_{mn}^{-1} \approx r^{-1} [1 - \mathbf{r} \cdot (\mathbf{R}_{mn} - \mathbf{r}) / r^2]$$

into Eq. (22), the first vanishes because of the Perelomov identity, Eq. (4), and the second term results in

$$w_{00}(\mathbf{r}) \approx - \frac{\mathbf{r}}{\sqrt{\pi\gamma} r^3} \sum_{mn=-\infty}^{\infty} (-)^{m+n} (\mathbf{R}_{mn} - \mathbf{r}) c_{mn}(\mathbf{r}). \quad (23)$$

The first factor in Eq. (23) falls off as r^{-2} , whereas the second is a periodic function of \mathbf{r} . If one plugs $\mathbf{r} = \mathbf{R}_{m'n'}$ in the second factor and applies Eq. (3), this factor takes the form:

$$(-)^{m'+n'+m'n'} \sum_{mn=-\infty}^{\infty} (-)^{m+n+mn} \mathbf{R}_{mn} c_{00}(\mathbf{r}).$$

The sum is equal to zero because of symmetry arguments, therefore, all lattice sites, $\mathbf{r} = \mathbf{R}_{mn}$, are zeros of the asymptotic expansion (23) of the function $w_{mn}(\mathbf{r})$.

It was shown by Kohn²⁷ that the rate of the falloff of an exponentially decaying Wannier function is determined by the distance of the singular point in the complex momentum plane from the real axis. In the problem of magnetic Wannier functions unavoidable singularities exist in the real (k_x, k_y) plane. These singularities result in the power-law falloff of the Wannier functions.

The asymptotic expansion of $K_\infty(m, n)$, Eq. (21), is accurate up to the values $|m|, |n| \approx 1$, e.g., the deviation of $K_\infty(1, 0) \approx -0.288$ from its approximate value following from Eq. (21) is only about 2%. The coefficient $K_\infty(0, 0) \approx 1.241$ is much larger than all the coefficients $K_\infty(m, n)$ with $m, n \neq 0$. One can subtract this large term and rewrite Eq. (22) in the form

$$w_{00}(\mathbf{r}) - c_{00}(\mathbf{r}) = \sum_{mn=-\infty}^{\infty} (-)^{m+n} \Delta(m^2, n^2) c_{mn}(\mathbf{r}), \quad (24)$$

The kernel $\Delta(m^2, n^2)$ is numerically small and can be considered as a smooth function of m and n . This allows the application of the arguments employed when deriving Eq. (23). Then the leading term in the right hand side of Eq. (24) vanishes because of the overcompleteness condition of Eq. (4). Therefore $w_{00}(\mathbf{r}) \approx c_{00}(\mathbf{r})$, which means that the difference between the functions $w_{00}(\mathbf{r})$ and $c_{00}(\mathbf{r})$ is expected to be small in the region where these functions are large. In the large r region, where these functions are small, $w_{00}(\mathbf{r})$ dominates and Eq. (23) should be used.

Numerical results support all of the above conclusions. The infinite-plane function $w_{00}(\mathbf{r})$ is shown in Fig. 2. Fig. 2a provides a detailed comparison of the shapes of the function $|w_{00}(\mathbf{r})|^2$ and the Gaussian function $c_{00}(r)^2$ in the region of $|x|, |y| \leq 1.5 \times \sqrt{2\pi}$. These functions are plotted along the x axis and along the diagonal, $x = y$, on the right and left hand sides of the figure, respectively. The function $w_{00}(\mathbf{r})$ is real on these lines. One can see that $w_{00}(\mathbf{r})^2$ and $c_{00}(r)^2$ are very close to each other in both directions. The function $w_{00}(\mathbf{r})^2$ shows small anisotropy: it is slightly elongated in the $x = y$ direction and squeezed in the x direction compared with $c_{00}^2(r)$. It is a remarkable property of the function $|w_{00}(\mathbf{r})|^2$ that it is very small in the points $\mathbf{r} = \sqrt{2\pi}(1, 0)$ and $\sqrt{2\pi}(1, 1)$. These points are the lattice sites adjacent to the origin. The suppression of $|w_{00}(\mathbf{r})|^2$ at the lattice sites of the two first

coordination spheres of the von Neumann lattice results in the squeezing of the central peak and a strong localization of $|w_{00}(\mathbf{r})|^2$. Consequently, the central region contributes about 95% to the normalization integral. The behavior of $w_{00}(\mathbf{r})$ along the x axis is shown in Fig. 2b over a wide region of x values. It is seen that $w_{00}(x, 0)$ oscillates and decreases with x . For $x \rightarrow \infty$, the oscillation amplitudes decrease as x^{-2} and zeros of $w_{00}(x, 0)$ approach multiples of the lattice period $\sqrt{2\pi}$ in agreement with Eq. (23). The exact $w_{00}(\mathbf{r})$ curve is almost indistinguishable from its asymptotic shape in the entire oscillatory region.

Therefore, functions $w_{mn}(\mathbf{r})$ show a two-scale behavior. The function $w_{00}(\mathbf{r})$ is large and shows only minor deviations from the Gaussian shape inside the central cell, but it is small, oscillates, and falls off according the r^{-2} law in the asymptotic region.

The set $w_{mn}(\mathbf{r})$ is orthogonal and complete by arguments of Sec. II. Therefore, any function which is invariant under the unitary transformations of the basis can be calculated in the Wannier representation. For instance, a straightforward calculation based on the representation of the functions $w_{mn}(\mathbf{r})$ through the kernel $K_\infty(m, n)$ and coherent functions $c_{mn}(\mathbf{r})$ shows that the function

$$C_\infty(\mathbf{r}, \mathbf{r}') = \sum_{mn=-\infty}^{\infty} \bar{w}_{mn}(\mathbf{r}) w_{mn}(\mathbf{r}') \quad (25)$$

is equal to the expression

$$C_\infty(\mathbf{r} - \mathbf{r}') = (1/2\pi) \exp\{-(\mathbf{r} - \mathbf{r}')^2/4\} \exp\left\{\frac{i}{2} \hat{\mathbf{z}} \cdot (\mathbf{r} \times \mathbf{r}')\right\}. \quad (26)$$

which can be also derived in the Landau representation. The last factor in Eq. (26) is gauge dependent. Therefore, the continuous symmetry of the magnetic translation group is recovered due to the completeness of the system $w_{mn}(\mathbf{r})$.

IV. SOME RESULTS FOR TOROIDAL GEOMETRY

Only few results can be obtained for Wannier functions $W_{mn}(\mathbf{r})$, Eq. (8), analytically. However, numerical methods allow one to study the dependence of $W_{mn}(\mathbf{r})$ on the plaquette

size (α, β) and the twist ϕ , and to check the self-consistency of the procedure. A number of results was obtained by Ferrari.^{6,23} The singular behavior of $\Psi_{\mathbf{k}}(\mathbf{r})$ near $\mathbf{k} = \mathbf{k}_0$ was studied in Sec. II.

In Fig. 3 the square of the modulus of the function $W_{00}(\mathbf{r})$ as well as the real and imaginary parts of $W_{00}(\mathbf{r})$ are shown for a square lattice with $\alpha = \beta = 3$ and $\phi = 0$. It is seen that $|W_{00}(\mathbf{r})|^2$ is nearly isotropic and well localized in the area of about $\sqrt{2\pi}$ near the origin. The shape of this function is close to the data⁶ for a triangular lattice. $\text{Re}\{W_{00}(\mathbf{r})\}$ is also rather isotropic and well localized, whereas $\text{Im}\{W_{00}(\mathbf{r})\}$ is small and highly anisotropic in the same region. The shape of the function $\text{Im}\{W_{00}(\mathbf{r})\}$ can be understood if one takes into account that, because of Eqs. (3) and (9), the expansion of $\text{Im}\{W_{00}(\mathbf{r})\}$ in the powers of z starts with the term $\text{Im}\{W_{00}(\mathbf{r})\} \propto \text{Im}\{z^4\}$. All lower-power terms cancel for a square lattice.

It is seen in Fig. 3 that all three functions possess full symmetry of the square lattice. For an odd-odd plaquette this high-symmetry shape appears only for the twist $\phi = 0$. When twist increases, the shape of $|W_{00}(\mathbf{r})|^2$ changes and becomes asymmetric. The changes are moderate near the maximum of the surface $|W_{00}(\mathbf{r})|^2$ but are considerably larger in its lower part. Dependence of the function $W_{00}(\mathbf{r})$ on ϕ becomes discontinuous when one of the points determined by Eq. (6) passes through the corner of the Brillouin zone \mathbf{k}_0 , since in the vicinity of \mathbf{k}_0 the function $\Psi_{\mathbf{k}}(\mathbf{r})$ critically depends on the phase φ_{ζ} of $\zeta = \mathbf{k} - \mathbf{k}_0$ as it follows from Eq. (16).

More generally, the function $|W_{mn}(\mathbf{r})|^2$ depends on ϕ discontinuously when i) both α and β are odd and $\phi_x = \phi_y = \pi$, ii) both α and β are even and $\phi = 0$, and iii) α is odd, β is even, and $\phi_x = \pi$ and $\phi_y = 0$.

Toroidal Wannier functions constructed by magnetic translations of infinite-plane functions $w_{mn}(\mathbf{r})$ have more stable shape than $W_{mn}(\mathbf{r})$. This approach will be discussed in more detail elsewhere.

It was shown in Sec. II that despite of the singular dependence of $\Psi_{\mathbf{k}}(\mathbf{r})$ and $W_{mn}(\mathbf{r})$ on the twist ϕ in the vicinity of \mathbf{k}_0 , these sets of functions remain complete at any values of ϕ .

The completeness can be checked by comparing the results obtained in the $W_{mn}(\mathbf{r})$ lattice basis with those in Landau function² basis. For example, the function

$$C(\mathbf{r}, \mathbf{r}') = \sum_{mn} \bar{W}_{mn}(\mathbf{r}) W_{mn}(\mathbf{r}') , \quad (27)$$

which is similar to the function $C_\infty(\mathbf{r}, \mathbf{r}')$, Eq. (25), does not depend on a specific choice of a complete basis set of the LLL. We have calculated the right hand side of Eq. (27) for finite plaquettes using both $W_{mn}(\mathbf{r})$ and Landau functions as given in Ref. 2. Gauge independent parts of $C(\mathbf{r}, \mathbf{r}')$ in both representations coincide with the accuracy of our computations. They were performed for the values of α and β up to 5. For the finite plaquettes the electron density $\rho(\mathbf{r}) = C(\mathbf{r}, \mathbf{r})$ oscillates with \mathbf{r} near its continuum limit $\rho_\infty = 1/2\pi$. The amplitude of oscillations decreases rapidly with increasing α and β . The number of oscillations in x and y directions equals the number of fluxes $\alpha\beta$ per a plaquette rather than the individual values of α and β , which are the number of lattice sites in corresponding directions. This property was found analytically in the Landau representation by Sutherland.²² It indicates disappearance of the pattern of the flux lattice and restoration of the symmetry of the underlying problem as it is expected since both periodic functions $W_{mn}(\mathbf{r})$ and Landau functions form complete sets. The completeness of the $W_{mn}(\mathbf{r})$ set is in agreement with the statements by Ferrari.⁶

V. CONCLUSION

The construction of infinite-plane localized magnetic Wannier-type functions was considered a challenging problem for a long time. It was shown that these functions, if they do exist, are subject to rigid restrictions. Three properties of a set of localized magnetic orbitals are incompatible: completeness, orthogonality, and exponential falloff.¹⁴ Moreover, for systems supporting a Hall current magnetic orbitals should fall off no faster than r^{-2} .¹⁵ The set of Gaussian coherent states on a von Neumann lattice violates these criteria because of the overcompleteness relation,¹⁰ which is a single linear constraint relating an infinite set

of orbitals. We believe that the complete set of orthogonal two-scale orbitals $w_{mn}(\mathbf{r})$ studied in this paper is the best compromise between the requirement of optimal localization and the inevitable restrictions on the degree of localization. Function $w_{00}(\mathbf{r})$ centered at the origin i) is large and possesses nearly Gaussian shape inside the region of the size of about $\sqrt{2\pi}l$ making a dominant contribution to the normalization integral, and ii) is small and falls off with a critical exponent r^{-2} outside this region. It is a striking property of the theory that the overcompleteness condition, Eq. (4), emerges and plays a crucial role at all stages of the derivation and study of the Wannier orbitals $w_{mn}(\mathbf{r})$.

We expect that $w_{mn}(\mathbf{r})$ orbitals form a convenient basis both for analytical and numerical calculations.

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FIGURES

FIG. 1. Normalization factor $\nu(\mathbf{k})$ for a square lattice.

FIG. 2. (a) Dependence of the functions $|w_{00}(\mathbf{r})|^2$ and $c_{00}(r)^2$ on r in the directions of the principal axes x and y (right) and the diagonals $x = \pm y$ (left). Solid line - $|w_{00}(\mathbf{r})|^2$, dashed line - Gaussian function $c_{00}(r)^2$. (b) Oscillatory dependence of the function $w_{00}(x, 0)$ on x . The exact solution, asymptotic solution, and envelope function proportional to x^{-2} are shown in the region $x \geq \sqrt{2\pi}l$ by solid, dotted and dashed lines, respectively.

FIG. 3. Shape of the function $W_{00}(\mathbf{r})$ for a square lattice with $\alpha = \beta = 3$ and $\phi = 0$. (a) - $|W_{00}(\mathbf{r})|^2$, (b) - $\text{Re}\{W_{00}(\mathbf{r})\}$, (c) - $\text{Im}\{W_{00}(\mathbf{r})\}$.











